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A Simple Advection Scheme for Material Interface (U)

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We introduce a new simple advection scheme for capturing multi-material interfaces. A material interface is tracked by solving a scalar transport equation of the volume of fluid. The method is developed by modifying the Hyper-C flux limiter and it does not require material interface reconstruction. A new single step unsplit advection scheme is developed by including corner flux monotonically. The algorithm is designed to minimize the necessary mixed zones as well as to preserve sharp and stable interfaces. Numerical tests show improvements compared to other existing methods such as Tipton's method. (U)

1. Introduction

A special technique is often used in Eulerian or ALE hydrodynamics to track the material interface accurately. One of the most popular methods in tracking the interface is based on the volume of fluid method. In the volume of fluid method, the volume fraction is assigned to each material and evolved by an advection equation. The interface is not explicitly tracked but can be constructed by using the volume fraction distribution. The accuracy of the method is dependent upon how the volume flux is calculated at the zone interface.

The first method for tracking the volume fraction was developed by Wilson and LeBlanc at LLNL around 1960 and is described by Bowers and Wilson(1991). Later, DeBar(1974) developed a different method based on interface reconstruction in his Eulerian hydrocode. The material interface is given by a single straight line and the slope of the line is determined by fitting straight line to give the correct volume fraction in the zone. A similar method was developed by Youngs(1982) and much effort has been spent to improve the method of interface reconstruction. On the other hand, the advection of volume fraction can be carried out by flux-limiting. This method does not require interface reconstruction and it is straightforward to extend the method to 3D and unstructured mesh. The development of this approach has been an active research area (Hirt and Nichols 1981, Tipton 1993, Lafaurie et al. 1994, Rudman 1997, Anninos 1999, Ubbink and Issa 1999). One of the most widely used algorithms at LLNL is the method developed by Tipton (1993). However, the method by Tipton has some weakness as well as many strengths. In this paper, we will develop a new method to overcome the limitations of Tipton's method.

There are several important requirements to make a good interface tracking algorithm: nondiffusiveness, accuracy, stability, symmetry, and mixed zone distribution. We will focus our attention on two important characteristics of the algorithm. First, floating mixed cells (floatsam and jetsam) should not be created. The problem concerning floating mixed cells is largely overlooked since the contour plot of volume fraction is often used to diagnose the quality of the interface advection scheme. So, the floating mixed cells away from the interface can be hidden. However, the floating mixed cells can cause problems such as perturbation to the flow. And advection of mixed zones is generally more expensive and less accurate than clean zone advection. One way to avoid the floating mixed cell is to set the volume fraction to zero if it becomes smaller than a predetermined small number. But this method can violate mass conservation severely. The second important issue is to preserve the interface shape stably. Under uniform advection, the interface should remain stable. The stability issue can be crucial in the study of fluid instability since small perturbations can change the developing fluid instability. Also, the lack of stability in the algorithm can be more problematic in low resolution such as poorly resolved thin shell as we will demonstrate in the next section. So, our goal is to develop a stable and nondiffusive method that does not creat unnecessary floating cells.

We will briefly describe the interface advection method by Tipton and explain its stength and weakness in Section 2. Then we will present our new method in Section 3. In section 4, the unsplit advection method is developed. The unsplit advection method is further developed for material interface in section 5. Finally, we will summarize in Section 6.

2. Tipton's Interface Advection Scheme

Tipton at LLNL has developed a new advection scheme for material interface by combining the Wilson-LeBlanc method and the SLIC method. The material flow is separated into parallel and series flow by calculating multi-dimensional slope. The advection of materials is done in a certain order. In series flow, the material has higher priority in advection if the volume fraction in the acceptor cell is greater than the volume fraction in the neighbor. On the other hand, the material has the lowest priority of advection if the volume fraction of the neighbor is greater than the volume fraction of the acceptor. In parallel flow, the second order term is included by taking into account the slope.

Figure 1 shows the numerical test results of four different methods on the Sandia balls and jacks problem. The entire computational domain($100cm \times 100cm$) is initialized on 100×100 mesh so that the thickness of crosses and circles is resolved with 3 cells. The initial advection velocity is 10.0 $cm/\mu sec$ in the diagonal direction and the density of crosses and circles is 2.78 and the background has the density, 1.0. The advection Courant number (vdt/dx) is taken as 0.5. Each plot shows the iso-contour of 0.5 volume fraction and mixed cell distribution represented by # at $t = 5.0\mu sec$. Each algorithm maintains the original shape of the material interface reasonably well. On the other hand, each plot shows very different result in the distribution of mixed cells. All four algorithms show mixed cells away from the interface although mixed cells should stay close to the material interface. Tipton's method produces the smallest number of mixed cells.

In the next test problem, we show a weakness of Tipton's method (Figure 2). The problem is designed by Gary Carlson at LLNL to test the capability for resolving the thin shell by the interface advection algorithm. The computational domain is resolved by 40 uniform zones and the shell in

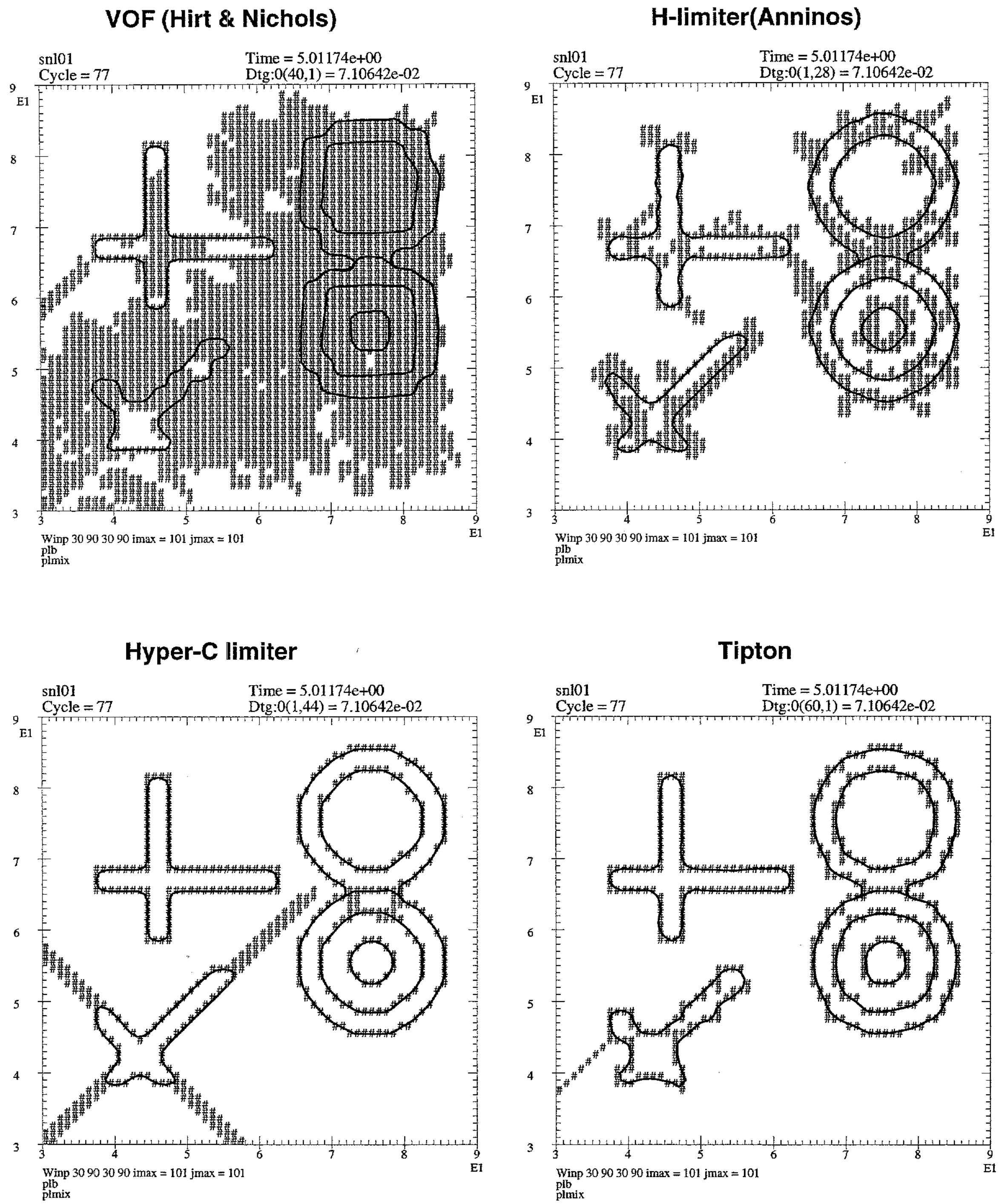

Figure 1: Numerical results of four different schemes on Sandia balls and jacks problem. (a) Volume of Fluid method by Hirt and Nichols, (b) H-Limiter method by Anninos, (c) Hyper-C limiter, (d) Tipton's method.

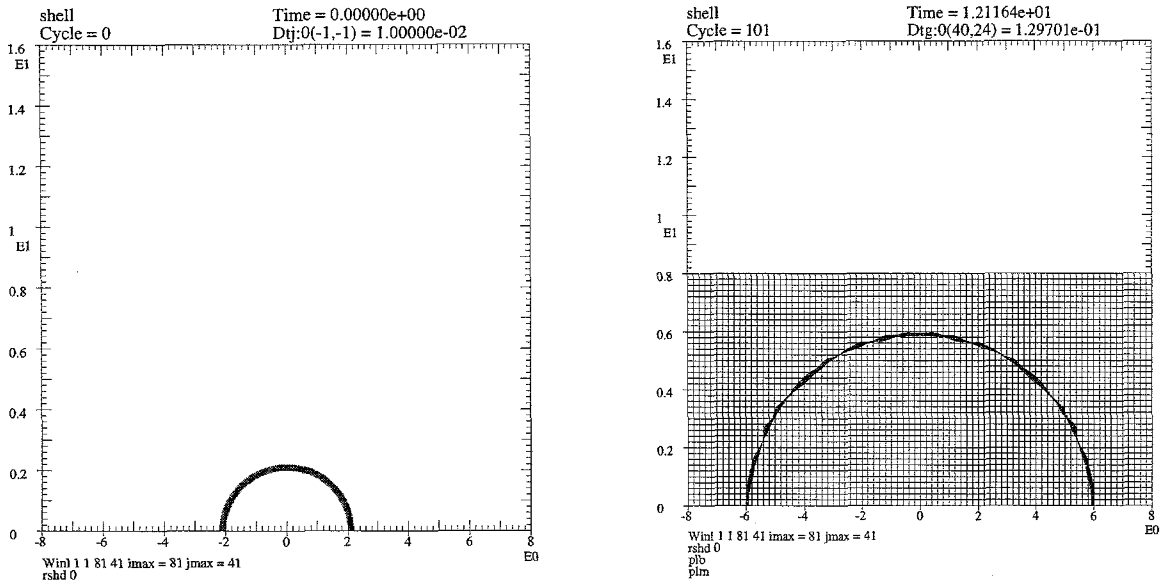

Figure 2: Expansion of thin shell by Tipton's method.

the middle region is only one zone thick. The background is initialized with $\rho = 0.01, e = 0.0001$ where ρ and e are density and internal energy, respectively. The thin shell and inner sphere are filled with hot gas of $e = 0.1$ and the inner sphere has higher density ($\rho = 1.0$) than the thin shell ($\rho = 0.1$). The equation of state for ideal gas is used with the adiabatic index, 1.4. The high pressure in the inner sphere and thin shell drives the outward expansion. The thin shell becomes thinner as it expands. The thin shell is shown to break into pieces and becomes disconnected. Although the thin shell is weakly unstable physically, the physical instability is not strong enough to grow significantly. In order to make sure that the shell breakage is the numerical defect of the algorithm, we ran the same calculation with higher resolution and found that the thin shell expanded stably and uniformly.

3. Modified Hyper-C Limiter for Mixed Zone Advection

In this section, we develop a new mixed zone advection method that can overcome the limitation of Tipton's method illustrated in the previous section. We construct the new method by modifying Hyper-C limiter (Leonard, 1991). Hyper-C limiter alone produces very good results in the expanding thin shell problem. However, as shown in Figure 1, Hyper-C limiter method can create many unnecessary floating mixed cells (jetsam, floatsam) away from the interface. So, our modification is necessary to remedy this problem.

First, we introduce the definition of Hyper-C limiter by two normalized volume fractions.

$$\tilde{f}_d = \frac{f_d - f_n}{f_a - f_n} \tag{1}$$

$$\tilde{f}_f = \frac{f_f - f_n}{f_a - f_n}. \tag{2}$$

where f_d, f_f, f_n, and f_a are volume fraction at donor cell, the interface between donor and acceptor cell, neighbor cell, and acceptor cell, respectively.

Then, Hyper-C limiter gives :

$$\tilde{f}_f = min(\frac{\tilde{f}_d}{c}, 1.0) : 0 \leq \tilde{f}_d \leq 1 \tag{3}$$

$$\tilde{f}_f = \tilde{f}_d : \tilde{f}_d < 0, \tilde{f}_d > 1 \tag{4}$$

where c is defined as normalized transfer volume, $\frac{dV}{V}$. Then, the transfer volume of material can be computed by

$$DV_m = min(f_f dV, f_d V_d, dV). \tag{5}$$

where DV_m is transfer volume of material through the cell face over the timestep, dV is total transfer volume, and V_d is donor cell volume.

In order to minimize the number of mixed cells to resolve the interface and avoid the creation of flotsam and jetsam, we add the following modification to the Hyper-C limiter:

$$DV_m = min(f_d V_d, dV) \quad if \quad (f_n < f_{small}) \quad \& \quad (f_d > f_a + f_{small}) \tag{6}$$

where f_{small} is typically 1.0e-10.

$$DV_m = min(f_d V_d, f_a dV, dV) \quad if \quad (f_n = f_a) \tag{7}$$

$$DV_m = 0.0 \quad if \quad (S > 1.0) \quad \& \quad (f_n > f_a) \tag{8}$$

where $S = \sqrt{\frac{(f_n - f_a)^2}{(f_{i,j-1,k} - f_{i,j+1,k})^2 + (f_{i,j,k-1} - f_{i,j,k+1})^2}}$. We note that the last modification [Eq. (8)] is also used in Tipton's method.

The next change is to advect materials in order by considering priority as used by Wilson-LeBlanc, Tipton, Anninos, etc. Materials are categorized into four groups according to the following rules.

$$Group1. \quad if \quad (f_n < f_{small}) \quad \& \quad (f_d > f_{small}) \quad \& \quad (f_a > f_{small})$$

$$Group2. \quad if \quad (f_n > f_{small}) \quad \& \quad (f_d > f_{small}) \quad \& \quad (f_a > f_{small})$$

$$Group3. \quad if \quad (f_n < f_{small}) \quad \& \quad (f_d > f_{small}) \quad \& \quad (f_a < f_{small})$$

$$Group4. \quad if \quad (f_n > f_{small}) \quad \& \quad (f_d > f_{small}) \quad \& \quad (f_a < f_{small}) \tag{9}$$

If more than one material falls to the same group, materials can be ordered further by calculating $P = \frac{f_a - f_n}{f_d}$. That is, material with higher P has higher priority.

The accumulated transfer volume of first n material (DV^n) is computed by taking accumulated volume fraction, $f^n = \sum_{m=1}^{m=n} f_m$. The individual material transfer volume can be obtained by

$$DV_m = max(0.0, DV^n - DV^{n-1}). \tag{10}$$

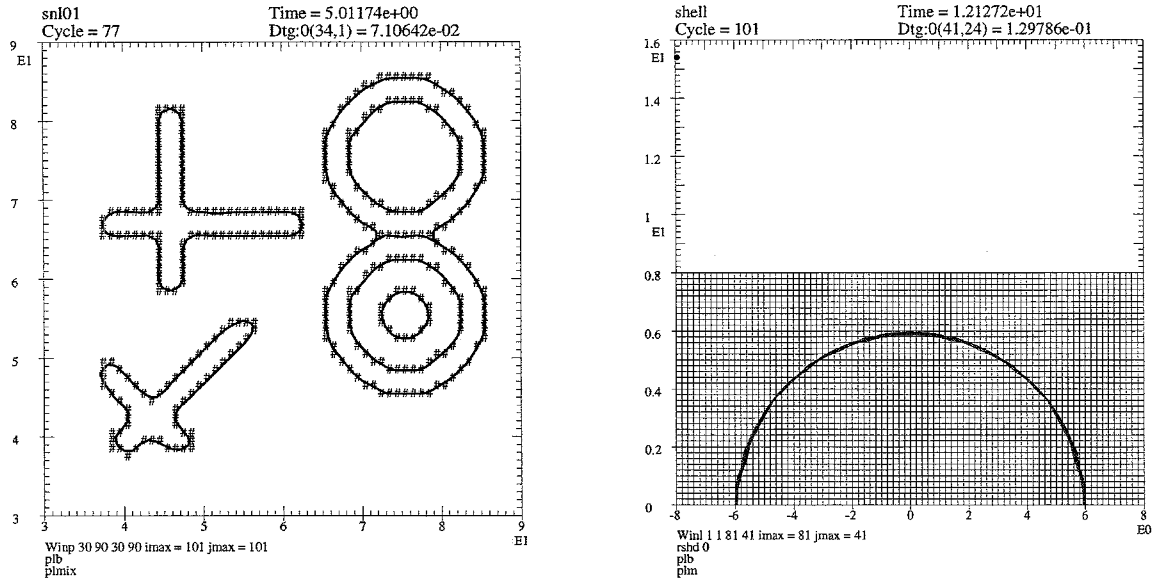

Figure 3: Numerical results of new mixed zone advection scheme. (a) Sandia balls and jacks problem. (b) Expanding thin shell problem.

And then we normalize each material by the total transfer volume of all material.

As shown in Figure 3, the new advection scheme produces considerably improved results. In the Sandia balls and jacks problem, all of the unnecessary floating mixed cells disappeared and the material interface was resolved by only one mixed zone. Besides, the original material shape is maintained well without much deformation. The result is also improved in the expanding thin shell test problem. The thin shell is well connected throughout its angular direction although the thickness of the shell is not quite uniform. This nonuniformity in the shell thickness resulted from the modification of Hyper-C limiter to avoid flotsam and jetsam. However, we will achieve further improvement by unsplit advection method in the next section.

4. Unsplit Advection

Single step unsplit advection is required for unstructured mesh or arbitrary connected structured mesh. Let us consider the scalar conservation law in two-dimensional space:

$$\frac{\partial f}{\partial t} + u \cdot \nabla f = 0 \tag{11}$$

where f is scalar variable. The explicit conservation form of the advection equation can be written as

$$f_{i,j}^{n+1} = f_{i,j}^{n} + \frac{u\Delta t}{\Delta x}(f_{i-1/2,j}^{n+1/2} - f_{i+1/2,j}^{n+1/2}) + \frac{v\Delta t}{\Delta y}(f_{i,j-1/2}^{n+1/2} - f_{i,j+1/2}^{n+1/2}). \tag{12}$$

where Δx and Δy are the zone width in x-direction and y-direction and Δt is the timestep.

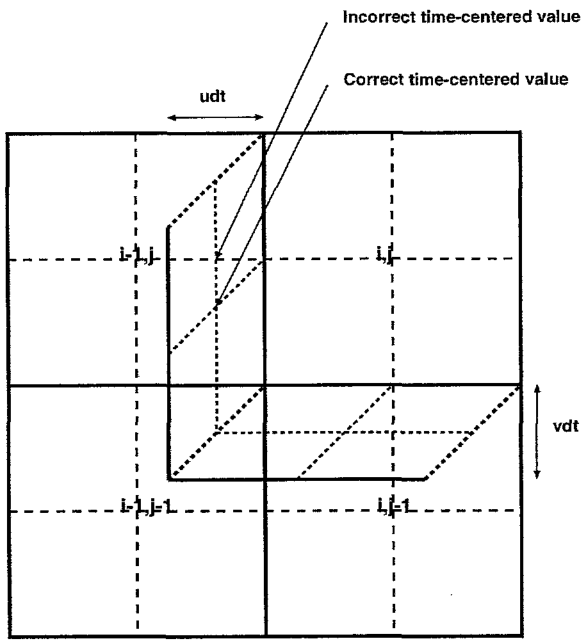

Figure 4: Correct time-centered face value in two-dimensional mesh.

The accuracy of scheme depends on how to calculate the time-centered value at the zone interface, $f^{n+1/2}_{i+1/2,j}$. The easiest way to calculate it is to use one-dimensional interpolation:

$$f^{n+1/2}_{i+1/2,j} = f^n_{i,j} + \frac{(\Delta x - u\Delta t)}{2}\frac{df}{dx} \tag{13}$$

This scheme turns out to be unsatisfactory. The contribution from the corner zone $(i-1, j-1)$ is not taken into account (Fig. 4) and it gives an incorrect time-centered value in two-dimensions.

Figure 5 shows advection tests of a two-dimensional ring. The initial condition is displayed in Figure 5(a). Initially, the background density is 1.0 and the ring density is 2.0. Both x and y components of advection velocity are 10.0. Figure 5(c) shows the result at t=6.0 by unsplit advection with one-dimensional interpolation. The shape of the ring is severely deformed compared to the split advection result in Figure 5(b).

Colella's CTU (Corner Transport Upwind) advection scheme includes the corner flux term:

$$f^{n+1/2}_{i+1/2,j} = f^n_{i,j} + (\frac{\Delta x}{2} - \frac{u\Delta t}{2})\Delta_x f_{i,j} - \frac{v\Delta t}{2\Delta y}(f^n_{i.j} - f^n_{i,j-1}). \tag{14}$$

where Δ_x is derivative in terms of x, that is $\Delta_x \equiv \frac{d}{dx}$. The last term is the flux in transverse direction (j). This scheme works reasonably well when van Leer's limiter is used for i-directional interpolation. But we find that the solution undershoots and overshoots if a steeper limiter such as superbee is used for interpolation as shown in Figure 6(a). Note that the initial density range was from 1.0 to 2.0. The maximum and minimum densities in Figure 6(a) are 2.034 and 0.8368. The scheme also suffers from severe deformation and loses initial shape information.

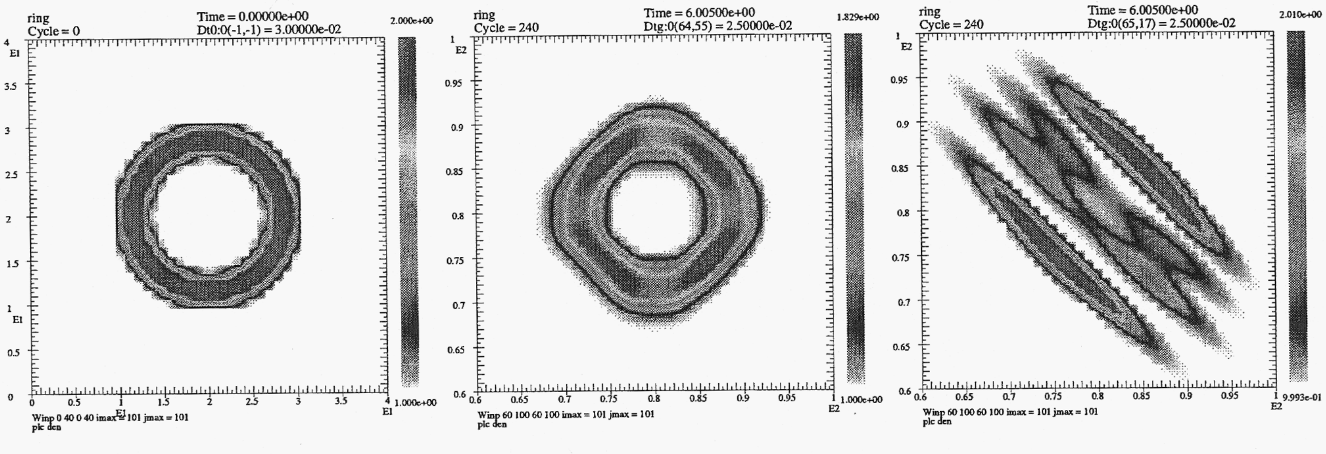

Figure 5: Advection tests of two-dimensional ring. (a): Initial condition, (b): directional operator splitting, (c): single step advection by one-dimensional interpolation.

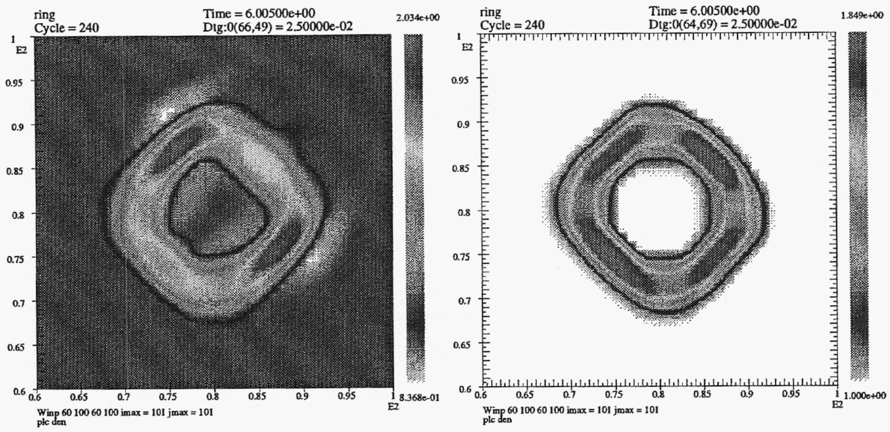

Figure 6: Advection tests of two-dimensional ring. (a): Colella's CTU scheme, (b): new unsplit advection scheme

In order to fix the problems of Colella's scheme, we modify equation (14) to write a new formula:

$$f^{n+1/2}_{i+1/2,j} = f^n_{i,j} + (\frac{\Delta x}{2} - \frac{u\Delta t}{2})\Delta_x(f^n_{i,j} - \frac{v\Delta t}{2}\Delta_y f) - \frac{v\Delta t}{2}\Delta_y f^n_{i.j} \tag{15}$$

The first change is done in the transverse flux term. While Colella's CTU scheme uses upwind slope, we find that the slope has to be obtained by the same interpolation method as the one used in i-direction. Therefore, both Δx and Δy are superbee slopes in our test. The second change is made to the i-directional slope calculation. We use the updated quantity by the transverse flux $(f^n_{i,j} - \frac{v\Delta t}{2}\Delta_y f)$ to compute the slope while Colella's scheme just uses the old quantity $(f^n_{i,j})$. The second change is critical to enforce the monotonicity not to allow undershooting and overshooting. The result by our new method shows significant improvement compared to the CTU scheme [Figure 6(b)]. The maximum (1.0) and minimum (1.849) densities are well within the initial range, 1.0 to 2.0.

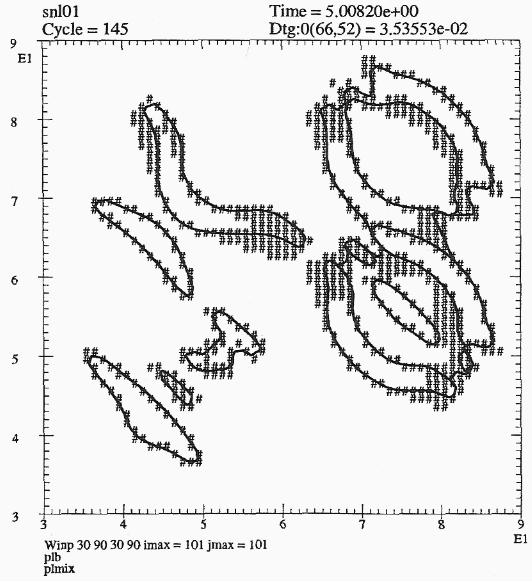

Figure 7: Single step advection of material interface without transverse flux term.

Our modified formula can be extended to three-dimensional ALE mesh:

$$f^{n+1/2}_{i+1/2,j,k} = f^n_{i,j,k} - \frac{dV_j}{2}\Delta_j(f^n_{i,j,k} - \frac{dV_k}{3}\Delta_k f^n_{i,j,k}) - \frac{dV_k}{2}\Delta_k(f^n_{i,j,k} - \frac{dV_j}{3}\Delta_j f^n_{i,j,k})$$

$$+\frac{V_i - dV_i}{2}\Delta_i(f^n_{i,j,k} - \frac{dV_j}{2}\Delta_j(f^n_{i,j,k} - \frac{dV_k}{3}\Delta_k f^n_{i,j,k}) - \frac{dV_k}{2}\Delta_k(f^n_{i,j,k} - \frac{dV_j}{3}\Delta_j f^n_{i,j,k})) \quad (16)$$

The term including $\frac{1}{3}$ factor represents far corner flux and the term including $\frac{1}{2}$ factor shows the near corner flux. We find that the far corner term is less important than the near corner term and can be ignored without noticeable loss of accuracy if computational cost is a concern.

5. Unsplit Advection of Material Interface

In order to track the material interface in an unstructured mesh, the volume fraction needs to be advected in single step symmetric fashion. The easiest way to achieve the symmetric advection is to compute the flux at the face of each cell by using one-dimensional interpolation. The numerical test of this method on the balls and jacks problem is shown in Figure 7. Tipton's interface advection scheme is used. As compared to Figure 1(d) that also uses Tipton's method in directionally split fashion, the material interface is severely distorted and many unnecessary mixed cells are created. This degraded result by single step advection is again due to the missing information from the corner zone. The transverse flux term can be included by using our modified corner transport scheme. The first step is to compute the slope of volume fraction in the transverse direction.

We define normalized volume fraction again as

$$\tilde{f}_i = \frac{f_i - f_{i-1}}{f_{i+1} - f_{i-1}} \quad (17)$$

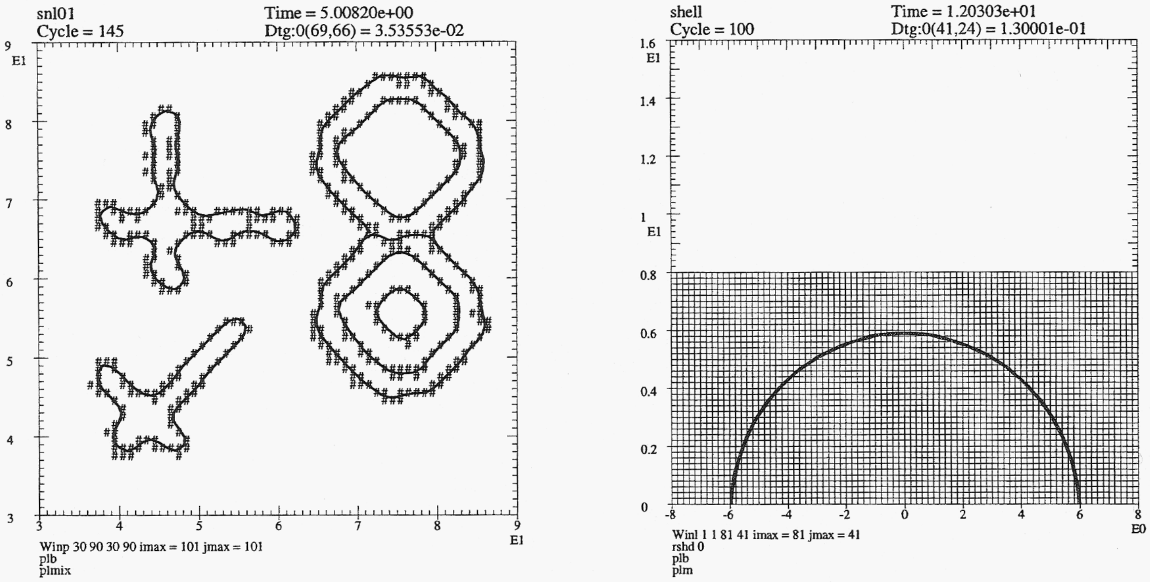

Figure 8: New unsplit advection of material interface. (a) Sandia balls and jacks problem. (b) Expanding thin shell problem.

Then, Hyper-C limiter gives:

$$\tilde{f}_u = min(\frac{\tilde{f}_i}{1.0 - c}, 1.0) : 0 \leq \tilde{f}_i \leq 1 \tag{18}$$

$$\tilde{f}_u = \tilde{f}_i : \tilde{f}_i < 0, \tilde{f}_i > 1 \tag{19}$$

where c is defined as $\frac{dV}{V}$ and f_i is the volume fraction at $i - th$ cell. Note $1.0 - c$ in the numerator instead of c here because zone-to-zone interpolation is carried out instead of zone-to-face interpolation.

Then, the slope in the transverse direction can be written as

$$\Delta f_{Hyper-C} = f_i - \tilde{f}_u(f_{i+1} - f_{i-1}) - f_{i-1} \tag{20}$$

We find that it is necessary to modify this Hyper-C limiter to avoid flotsam and jetsam as follows.

$$\Delta f_1 = (f_i - f_{i-1})(\frac{dV}{V_i + V_{i-1}}),$$

$$\Delta f_2 = (f_{i+1} - f_i)(\frac{dV}{V_i + V_{i+1}})$$

$$\Delta f_{min} = min(\Delta f_1, \Delta f_2) \tag{21}$$

Then the slope in the transverse direction is

$$\Delta f = \Delta f_{min} : \tilde{f}_i < 0.15, \tilde{f}_i > 0.8 \tag{22}$$

$$\Delta f = \Delta f_{Hyper-C} : otherwise \tag{23}$$

The numerical results of new unsplit advection of material interface using modified Hyper-C limiter are shown in Figure 8. The material shape of Sandia balls and jacks problem is maintained better and the number of floating mixed cells is decreased [Figure 8(a)]. Figure 8(b) shows the test result of expanding thin shell problem with the new method. The thin shell expanded uniformly and stably. The uniformity of the thin shell is greatly enhanced as compared to the result by directionally split method (Fig. 3).

6. Summary

We have developed a new method for material interface advection by modifying Hyper-C limiter in two- and three-dimension. We have also developed unsplit advection method of material interface by including corner transport term. The method does not require explicit reconstruction of the interface and is easy to implement in a hydrocode. Numerical tests show improvements compared to other existing methods such as Tipton's method.

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